Vibration of Nonhomogeneous Square Plate with Circular Variation in Density

Amit Sharma

Abstract Here, an analysis of vibrational frequency of nonuniform and nonhomogeneous square plate is presented. In view of nonuniformity and nonhomogeneity in plates material, the author considered linear variation in thickness and circular variation in density. The variation of temperature is assumed bilinear (linear along both axes). To analyze the behavior of frequency modes under different variations in parameters, Rayleigh–Ritz technique is used.

1 Introduction

The failure of structures and noise are caused because of excessive dynamic behavior. To increase the safety and reliability of structures, it is required to have a better understanding of dynamic properties of structures. To do modal analysis of structures, it is essential to calculate natural frequencies and mode shapes. These parameters play an essential role in the designing of structures and determine the dynamic characteristics of existing structures.

Plates are very common components (structural), which have been widely applied in various applications of engineering and sciences, viz., civil engineering, aerospace engineering, ocean engineering, optical instruments, etc. Numerous studies have been carried out to analyze the characteristic of plates.

Chopra and Durvasula [1] provided frequency (natural) of vibration with mode shape of symmetric trapezoidal plate on simply supported condition. Free vibrations of rectangular (viscoelastic) tapered (linear variation in thickness) plate have been discussed by Gupta and Khanna [2]. Hutchinson and Zillmer [3] applied series solution and determined accurate natural frequency of vibration of rectangular parallelepiped having transaction-free surface. Rayleigh–Ritz method has been applied by Itakura [4] to analyze natural vibration of skewed plate with arbitrary boundary conditions. Khanna et al. [5] studied the behavior of temperature and exponential

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SYNERGISTIC IMPACT OF IRON (III) OXIDE NANOPARTICLES AND ORGANIC WASTE ON GROWTH AND DEVELOPMENT OF *SOLANUM LYCOPERSICUM* PLANTS: NEW PARADIGM IN NANOBIOFERTILIZER

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Abstract

Nanoparticles have shown a significant effect in plant growth and crop production when used as fertilizers alone or in combination with other biofertilizers. The combination of Iron (III) oxide (Fe_2O_3) nanoparticles with flower waste and cow-dung showed significant enhancement in the growth of tomato plants compared to other fertilizers used. Student's t-test provided statistical significance under different combinations of fertilizers. After analyzing the growth of tomato plants over several weeks under these different fertilizers, it is concluded that Fe_2O_3 nanoparticles could be very useful as a component of new generation eco-friendly nanobiofertilizers, without having usual toxic and environmental risk factors that are associated with existing conventional chemical fertilizers.

Key words: Nanobiofertilizer, Iron (III) oxide (Fe_2O_3) Nanoparticles, biocompatibility, waste-derived fertilizer

Introduction

Over the last two decades, nanoparticles have found extensive application in diverse fields starting from electronics to energy, and medicine to life sciences (Giraldo *et al.*, 2014). Nanotechnology plies an expanding paradigm to specific research areas, such as reproducing biology, organic wastes converted into energy (Singh and Usha 2014; Zhang *et al.*, 2017) and other beneficial by-products through enzymatic Nano-bio-processing, chemical sensors, water treatment, prevention of diseases, and plant treatment by the use of various nanocides (Moraru *et al.*, 2003). A huge percentage of applied nutrients remain unavailable to plants due to the factors like leaching, photolytic breakdown, hydrolysis and decomposition (Bentley 1948). Hence, the current situation demands lessening in nutrient loss and increasing the crop yield by using fertilizers. One of the possible routes to surpass this problem is the use of novel bio-fertilizers having nanoparticles as one of the compositions. Nano-encapsulated nutrients and/or Nano-bio-fertilizers

may have characteristics that can intensify crop yield in food crops mainly vegetable crops, timely release of nutrients by which plant growth is regulated, and targeted activity is enhanced (DeRosa *et al.*, 2010). Higher plants can acquire a mechanism to cope up with favorable and unfavorable conditions. Nowadays scientists/researchers are looking for new techniques that can enhance the native functions of plants. Nanoparticles with their unique physico-chemical properties can boost up the plant metabolism (Yuvakkumar *et al.*, 2011). Engineered nanoparticles have the potential to get inside plant cells and leaves by acting as chaperones for transporting genetic materials and chemicals (Galbraith 2007; Lin and Xing 2007). This area of research generates new possibilities in environmental sciences as well as in plant biotechnology (Siddiqui *et al.*, 2015). There are reports of enhancement of plant's capability to capture more light by targeted delivery of carbon nanotubes (C-nanotubes) into the chloroplast. The C-nanotubes can also aid as artificial antennae that allow chloroplast to harvest light of unusual wavelength like ultraviolet, green, and near-infrared

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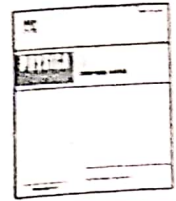
Investigation of structural and optical properties of ZnO thin films of different thickness grown by pulsed laser deposition method

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ABSTRACT

In this paper, we investigated the effect of film thickness on structural, surface morphology and optical properties of ZnO thin films grown by pulsed laser deposition (PLD) method. Thickness of the films was varied by keeping all other PLD parameters same to investigate thickness dependence on the structural and optical properties of ZnO thin films. The prepared thin films have been characterized by X-ray diffraction (XRD), atomic force microscopy (AFM), UV- visible (Uv–Vis) and photoluminescence (PL) spectroscopy. XRD confirms the formation of crystalline c-axis orientated hexagonal wurtzite structure of ZnO thin films. AFM depicts that roughness and grain size of the ZnO films increase with increase in the films thickness. The direct optical band gap of the ZnO films calculated using Tauc's plot increase from 3.28 eV to 3.34 eV as the thickness of the films varies from 55 nm to 220 nm. The high quality c-axis orientated ZnO thin films with minimum strain and tuneable optical properties could be used as a transparent conducting oxide (TCO) for optoelectronic applications.

1. Introduction

During the last several decades, wideband gap semiconductors have received great interest from the scientific community due to their potential applications [1,2]. Zinc oxide (ZnO) is a promising semiconductor material from II-VI group with a wide energy band gap (~3.37 eV), having a stable hexagonal wurtzite crystal structure and free excitons binding energy (~60 meV) at room temperature [3]. The promising properties make ZnO as a superior material for various applications in optoelectronics, light emitting device, transducers, solar cells, photocatalytic, transparent conducting contact, spintronic devices and gas sensors [4–7]. Also, the occurrences of both high optical transmittance in visible region and lower resistivity prompt the ZnO as potential material in fabrication of heat mirrors used in gas stoves and the conducting coating in mirror used in aircraft to avoid the icing [8,9]. Many of these applications are based on coexisting occurrences of high transmittance and low resistivity in the visible region, when ZnO is synthesized in the form of thin films. The tuning of the physical properties of ZnO by doping is a challenging task while fabricating the devices [10,11].

The fundamental properties of ZnO thin films depend upon the deposition methods and various parameters. Various synthesis methods such as thermal evaporation [12] RF magnetron sputtering [8] sol-gel method [13] chemical bath deposition [14] chemical vapor deposition and pulse lase deposition method (PLD) have been widely used to prepare the ZnO thin films [15,16]. Among all the above methods PLD method is a promising technique for growing the high quality ZnO thin films with the high adhesive quality. This technique has the potential to transfer the stoichiometry of target material to substrate by striking the target materials by high kinetic energy of laser beam during the deposition process in comparison of other Physical deposition (PVD) methods [17,18]. This method is suitable to deposit the films with the required properties for optoelectronic applications by controlling various synthesis parameters. Therefore, the present study is dedicated to investigate the structural, morphological and optical properties of PLD deposited ZnO thin films. As the application of ZnO in optoelectronics device, normally the optimum film thickness is required for best device performance. Therefore, it is highly motivating to the study the effect of

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Enhanced near-band edge emission in pulsed laser deposited ZnO/c-sapphire nanocrystalline thin films

Veeresh Kumar[1] · Himanshu Sharma[1] · Shushant Kumar Singh[1] · Shalendra Kumar[2] · Ankush Vij[3]

Abstract

We report on the enhanced near-band edge emission with negligible defect-assisted emission in ZnO nanocrystalline thin films of varying thickness on c-sapphire substrates. X-ray diffraction studies reveal wurtzite structure of thin films grown preferentially along (002) plane. The crystallinity and grain size of the deposited films have been increased with increase in film thickness. The band gap of the films was calculated by Tauc's plot which shows negligible change in band gap with increase in thickness of ZnO film. The various Raman modes observed in ZnO thin films of different thicknesses support the formation of hexagonal wurtzite structure. The room temperature photoluminescence (PL) spectrum shows the strong near-band edge emission in the wavelength range 378–381 nm which further enhances with film thickness. The enhanced PL emission in near ultraviolet visible (UV) region with negligible defect-assisted emission may find potential applications in ZnO-based UV-excited light-emitting diodes.

1 Introduction

Zinc oxide (ZnO) is a (II–VI) group compound semiconductor with a wide direct band gap (3.4 eV) and has a stable hexagonal wurtzite crystal structure [1, 2]. ZnO-based nanostructures have attracted researchers due to its extraordinary properties and versatile applications in transparent electronics [3], ultraviolet light emitters [4], piezoelectric devices [5], chemical sensors [6] and spin electronics [7]. The large exciton binding energy (60 meV) of ZnO makes it more promising material for UV-emitting phosphor in comparison to the gallium nitride (GaN) [8]. The large exciton binding energy of the ZnO also leads to reduced UV lasing threshold

at room temperature and yield the higher UV-emitting efficiency [9]. As a wide gap semiconductor, ZnO is more promising element for optoelectronic devices such as laser diodes (LDs), blue to UV light-emitting diodes (LEDs) and white light emitters by phosphors excitation with important applications in solid-state lighting and for high-density data storage devices [4, 10]. The higher transparency of ZnO in visible light provides the opportunity to manufacture the transparent electrode, UV optoelectronics and integrated sensors and makes ZnO an excellent choice for transparent front electrodes in solar cells and displays [11, 12]. There are various methods to synthesize the ZnO thin film such as sol–gel method, RF sputtering, spin coating, dip coating, electron beam deposition, and pulse laser deposition [13–17]. Among all these methods, pulsed laser deposition (PLD) technique is unique to grow the high-quality film with good control over the depth as well as high adhesion with the substrate. In PLD technique, the pulsed laser beam strikes the target material and transfer the target composition to the substrate. The plasma generated by the pulsed laser beam is very energetic and density of the plasma plume can be easily controlled by varying the oxygen pressure. There are various reports on the variation of different parameters on ZnO thin films deposited by PLD techniques. Jin et al. [18] have reported that ZnO thin films deposited on the sapphire substrates at three different temperatures 200 °C, 300 °C and 400 °C exhibit the photoluminescence (PL) in violet

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Electronic Structure and Room Temperature Ferromagnetism in Gd-doped Cerium Oxide Nanoparticles for Hydrogen Generation via Photocatalytic Water Splitting

Swati Soni, Neelu Chouhan, Rajesh Kumar Meena, Sudhish Kumar, Bhavna Dalela, Monu Mishra, Rajendra Singh Meena, Govind Gupta, Shalendra Kumar, Parvez Ahmad Alvi, and Saurabh Dalela*

Enhanced visible light photocatalytic activity of Gd-doped CeO_2 nanoparticles (NPs) is experimentally demonstrated, whereas there are very few reports on this mechanism with rare earth doping. All-pure and Gd-doped CeO_2 NPs are synthesized using a coprecipitation method and characterized using X-ray diffraction (XRD), absorption spectroscopy, surface-enhanced Raman Spectroscopy (SERS), X-ray photoelectron spectroscopy (XPS), and superconducting quantum interference device (SQUID). The effect of Gd-doping on properties of CeO_2 is discussed along with defects and oxygen vacancies generation. The XRD confirms the incorporation of Gd^{3+} at the Ce^{3+}/Ce^{4+} site by keeping the crystal structure same. The average particle size from transmission electron microscopy (TEM) images is in the range of 5–7 nm. The XPS spectra of Ce 3d, O 1s, and Gd 4d exhibits the formation of oxygen vacancies to maintain the charge neutrality when Ce^{4+} changes to Ce^{3+}. The gradual increase in hydrogen production is observed with increasing Gd concentration. The observed results are in good correlation with the characterization results, and a mechanism of water splitting is proposed on the basis of analyses. The absorption spectra reveal optical band gap (2.5–2.7 eV) of samples, showing band gap narrowing leads to desired optical absorbance and photoactivity of NPs.

1. Introduction

Rare earth (RE) oxide-CeO_2 has attracted great interest of research due to their unique properties, including high oxygen storage capacity and ability to uptake and release oxygen (O^{2-}) ions via conversion of oxidation state of cerium ion from Ce^{4+} to Ce^{3+}, due to formation of defect space, such as oxygen vacancies in the lattice, of CeO_2.[1] On account of this uniqueness, CeO_2 has been widely used as three-way catalysts for eliminating vehicle exhaust gases,[2] UV blocker materials in sunscreens, UV-shielding used in cotton fabrics,[3] functionalize silk fiber for antibacterial activity,[4] oxygen sensors,[5] and oxygen ion conductors in solid oxide fuel cells (SOFCs).[6] Generally, it has been reported that, type of dopant strongly influenced the electrical properties of ceria and high conductivity at low temperature is an essential requirement for SOFCs, therefore, rare earth (RE)-doped cerium oxide, $Ce_{1-x}RE_xO_{2-\delta}$ (RE = Sm,

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Band gap engineering, electronic state and local atomic structure of Ni doped CeO$_2$ nanoparticles

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Abstract

In cerium dioxide (CeO$_2$) as semiconductor compound, the tuning of band gap energy is a pivotal feature for visible light applications. In this report, nanoparticles (NPs) of Ce$_{1-x}$Ni$_x$O$_2$ (0.0 ≤ x ≤ 0.10) were synthesized through co-precipitation route. The structural, electronic state and optical band gap were investigated by means of X-ray diffraction (XRD), transmission electron microscopy (TEM), near edge X-ray absorption fine structure (NEXAFS) spectroscopy, Raman scattering and UV–Vis spectroscopy. XRD results revealed the single-phase nanocrystalline behavior of CeO$_2$ with cubic fluorite structure. The electronic configuration of the samples, probed via NEXAFS spectra at Ce M$_{5,4}$ edges, demonstrated that the cerium exists in Ce^{4+} and Ce^{3+} mixed valence states. The formation of Ce^{3+} ions in the vicinity of oxygen vacancies (Ov) were assessed also via Raman scattering and XANES spectra at Ce L$_3$ edge. The estimated concentrations of Ce^{3+} were increased from 6 to 13% as the Ni content increase from 0 to 10% respectively. Here, the inclusion of Ni^{2+} ions into CeO$_2$ network induced additional Ov and simultaneously reduced the optical band gap from 3.9 eV for pure CeO$_2$ to 2.6 eV for 10% Ni doped CeO$_2$ NPs. Therefore, the oxygen loss population seem to be responsible for the band gap reduction. The role of Ov for creating profound donor band near the conduction band and narrowing the band gap energy were discussed.

1. Introduction

Nanostructured metal oxide semiconductors (SnO$_2$, ZnO, TiO$_2$, CeO$_2$ etc) have gained immense eminence in the province of material science because of their wide range of technical application. Ceria (CeO$_2$) as compound semiconductor has attracted a significant attention due to its specific properties like oxygen storage capacity, small band gap energy, which make it suitable for various modern-day devices like gas sensors, high storage capacitor devices, solid oxide fuel cells, ultra-fast optical switches, polishing materials and

UV-absorbent, etc [1–4]. The unique feature of CeO$_2$ that makes it worthwhile is its functional ability to undergo oxidation and reduction processes through which it releases or stores oxygen. Interestingly, while doing so, CeO$_2$ upholds its cubic fluorite structure by enduring the stoichiometric deviations [4]. This suggests that the oxygen present in the configuration of CeO$_2$ lattice is more susceptible to the oxidation/reduction conditions, which turns it to be one of the most active redox binary metal oxides. The redox cycle (Ce^{4+} ↔ Ce^{3+}) enhances the photochemical activity of ceria and converting the sun light into sustainable and harmless source of energy in solar cell (photovoltaic).

Many groups of researchers have put great endeavors to comprehend the origin of Ov and how the oxygen loss population alters the properties of CeO$_2$ NPs. They are striving to find ways and means to improve the electronic structural, magnetic, optical and catalytic properties of the materials [5–11]. Dutta et al. have pronounced that the weakly bound oxygen atoms are responsible for creating holes i.e. oxygen vacancies in the CeO$_2$ lattice [2]. Adaptation in the material-properties is subject to the synthesis and environmental conditions yet many methods and techniques have been explored and refined to enhance their properties. One such method is to dope CeO$_2$ with few percentages of some

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High pressure affects on optical characteristics of AlGaAs/GaAsP/AlGaAs nano-heterostructure

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ABSTRACT

This paper gives a detailed report on the tunability of optical gain characteristics of type-I n-$Al_{0.45}Ga_{0.55}As/GaAs_{0.84}P_{0.16}/p-Al_{0.45}Ga_{0.55}As$ nano-scale hetrostructure under the external pressures applied along [001] and [100] directions. In order to find the carriers wavefunctions, their localizations and sub-band dispersions in the heterostrcuture, a 6 × 6 K –L Hamiltonian was solved. In addition, the optical and momentum matrix elements were also calculated followed by the calculation of TE and TM optical gain under the applied pressure along [001] and [100] directions. According to the quantitative analysis of the simulated results, it can be suggested that the application of external pressure along [001] direction within TE mode is one of the preferable approaches for the efficient improvement in the gain characteristics of the n-$Al_{0.45}Ga_{0.55}As/GaAs_{0.84}P_{0.16}/p-Al_{0.45}Ga_{0.55}As$ nano-scale hetrostructure based laser performance in the NIR (near ifrared region).

1. Introduction

Heterostructures are an integral part of modern solid state physics based opto-devices. The leading edge of semiconductor electronics has explored the heterostructures very well due to their impending applications and usage in various optoelectronic devices [1–3]. For the purpose of applications in optoelectronic communication, some particular material systems based hetero-structures, such as InGaAlAs/InP, and InGaAsN/InP heterostructures have been very popular [4–6]. These heterostructures have been found to show peak optical at 1.55 μm and 1.30 μm, respectively. For these heterostructures, gain suppression has also been calculated and shown in references [5,6]. The main reasons behind the gain suppression are spectral hole burning and carrier heating. It is stronglly depend on material in the active region. Theoretical studies shows that strained quantum well (QW) laser present enhanced carrier effects. By introducing electrons into the lasing subband of the active region (quantum well) at or near the fermi level via tunneling, the hot carrier effects can be minimized. The designing of laser has raised several issues. The primary issue is to generate a population inversion (generation of sufficiently high population of atoms in excited state). In solid state semiconductor lasers, population inversions are brought out by intoducing impurity within a host material and then exciting them with suitable light

Investigation of local geometrical structure, electronic state and magnetic properties of PLD grown Ni doped SnO_2 thin films

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ABSTRACT

We have investigated the ferromagnetic behavior, electronic states and local geometrical structure of Ni (2 and 10 at %) doped SnO_2 thin films. The films were successfully fabricated with the help of pulsed laser deposition (PLD) technique on Si (100) substrate under ultrahigh vacuum (UHV) condition. X-ray diffraction (XRD) results revealed the single phase character of SnO_2 rutile lattice structure with $P4_2/mnm$ space group. The inclusion of Ni ions into SnO_2 matrix induced oxygen vacancy (Vo), enhanced the distortion in octahedral local symmetry and reduced the oxidation state of the host Sn^{4+} (SnO_2) to Sn^{3+} (Sn_2O_3), these details have been estimated by Raman scattering, Near edge X-ray absorption fine structure (NEXAFS) spectra at Ni $L_{3,2}$ and O K edges. Further quantitative details on the local geometrical structure around Ni ions were obtained via fitting the experimental Fourier transforms EXAFS spectra $|X(R)|$ with FEFF6 code. The magnetization measurements performed at room temperature (RT) infers that Ni doped SnO_2 films displayed ferromagnetic (FM) signal, and there was no significant difference in the saturation moments even with increase in the Ni content. Hence, the similarity in the observed magnetic behavior of the films seems relevant to the same crystal growth condition (UHV) and might not be limited directly to the Ni dopant concentrations. The FM signal and the role of surface defects have been discussed in the light of spin-split impurity band percolation mechanism.

1. Introduction

The oxides based diluted magnetic semiconductors (DMSs) have been studied extensively because of their potential use in innovated spintronic devices. The operation of such devices would be tuned by coupling the spin and charge of electron, simultaneously, with an external magnetic field. Thereby, the ferromagnetic (FM) ordering with Curie temperature far in excess of 300 K is a fundamental requirement DMS materials to be used in future spintronic technology [1–6]. Among the variety of DMS materials, like CeO_2, TiO_2, ZnO and etc, tin dioxide (SnO_2) has attracted significant attention because of its specific properties and application, i. e., its visible light transparent character, due to its wide band gap energy ($E_g = 3.6$ eV), is an important aspect for the possible application in spin-dependent optoelectronics [6,7]. The Frenkel defect of oxygen vacancies present naturally near the surfaces of SnO_2, due to lack of nearest neighbors at the outer boundaries, causes a reduction in the oxidation state of partial SnO_2 (Sn^{4+}) to Sn_2O_3 (Sn^{3+}). So, SnO_2 possesses reversible valence states and easy redox cycle ($Sn^{4+} \leftrightarrow Sn^{3+}$) like other metal oxide CeO_2 ($Ce^{4+} \leftrightarrow Ce^{3+}$) or TiO_2 ($Ti^{4+} \leftrightarrow Ti^{3+}$). Therefore, SnO_2 is considered as redox binary metal-oxide with high photochemical activities for potential application in solar cell, photocatalyst activity, oxygen gas sensors and oxygen storage, etc [8,9].

Dilution of SnO_2 host semiconductor by magnetic transition metal (TM) elements as DMS system have been studied widely and great efforts have been paid for comprehension the source of FM signal in DMS systems, but still there is a controversial issue in such types of materials [10]. In most recent reports, there is a consensus on the importance of surface defects to drive the ferromagnetic response, but the exact mechanism is not yet clear. In spin-split impurity band percolation

Cosmology using long gamma-ray bursts: statistical analysis of errors in calibrated data

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Abstract We investigate direction dependence and non-Gaussian features in high-z cosmological data using Δ_{χ^2} and Δ_χ statistics and the Kolmogorov-Smirnov test. These techniques are applied on a set of calibrated long gamma-ray bursts (GRBs) and its combination with recent Type Ia supernovae data (Union2). Our statistical analysis shows a weak but consistent direction dependence in both the data sets. The analysis also indicates a non-Gaussian nature of errors in both data sets.

Key words: gamma-ray bursts — observational cosmology — cosmological parameters — Gaussian distribution — supernovae

1 INTRODUCTION

Gamma-ray bursts (GRBs) are among the most energetic explosions in the Universe. Their high energy photons in the gamma-ray band are almost unaffected by dust extinction, and as a result they are detectable up to very high redshifts (Salvaterra et al. 2009; Cucchiara et al. 2011). Long GRBs (for which pulse duration is greater than 2 s) can be used to investigate the Universe at high redshifts, which is difficult to access by Type Ia supernovae (SNe Ia); thus long GRBs have been proposed as a complementary probe to SNe Ia. However, due to an extensive variety of isotropic equivalent luminosities and energy outputs (Ghirlanda et al. 2006), GRBs cannot be treated as standard candles. Efforts have been made to calibrate long GRBs using the following empirical relations:

- Isotropic equivalent radiated energy (E_{iso}) and peak energy (E_p) correlation for GRBs (Amati et al. 2008).
- Peak energy (E_p) in vFv spectra and collimated emission (E_γ) correlation for GRBs (Ghirlanda et al. 2004).

Unfortunately, physical interpretation of the above correlations is not well understood. Thus, standardization

of these correlations is subject to availability of low redshift GRBs. Since not many low redshift GRBs are available (Kodama et al. 2008; Li et al. 2008), the calibration is obtained by assuming a specific cosmology (specific values of cosmological parameters). As a result, the GRB data obtained from this calibration depend on cosmology, and hence cannot be further used for estimation of cosmological parameters. This problem is known as the "circularity problem" in GRB cosmology. It should be noted that while deriving distances to SNe Ia, sometimes the numerical value of the Hubble constant is inserted by hand (Amanullah et al. 2010) which makes it cosmology-dependent. However, one can easily overcome this problem by making use of nearby SNe Ia.

In order to use GRBs as cosmological probes, one needs specific statistical techniques to avoid the circularity problem. Many cosmology-independent methods have been proposed to achieve this, e.g., the collimation-corrected energy method (Ghirlanda et al. 2004), the luminosity indicator method (Liang & Zhang 2005) derived from 157 SNe Ia, the Bayesian method (Firmani et al. 2005) and the Markov Chain Monte Carlo (MCMC) method (Li et al. 2008). Recently Liu & Wei (2015) have used the Padé approximation to calibrate high-redshift

Natural vibration of tapered rectangular plate with exponential variation in non homogeneity
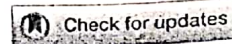
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Abstract. In this paper, authors studied the natural vibration of tapered non homogeneous rectangular plate on clamped edges. For tapering in plate, authors considered circular variation in thickness and for non-homogeneity (in plate's material) Poisson's ratio varies exponentially. Bilinear temperature (linear along both the axes) variation on the plate is being viewed. Rayleigh Ritz method is used to solve differential equation of motion. All the results are presented with the help of tables and graphs. A comparison of results is also given to support the present study.

Keywords: rectangular plate, exponential variation, natural vibration, non homogeneity.

1. Introduction

The non uniform and non homogeneous rectangular plate are used in various engineering structures such as aerospace engineering, marine engineering, ocean engineering, optical instruments and mechanical engineering. Non uniform and non homogeneous plates have greater efficiency when compared to uniform and homogeneous plates because of reduction in weight, high tensile strength, durability, elastic behavior and size. The study of plate vibration without consideration of temperature is nothing because almost all engineering structure worked under great influence of temperature. Thus, to design an accurate structure, determination of natural frequencies and mode shape are essential. A significant work has been provided in these directions.

Timoshenko and Woinowsky-Krieger [1] discussed comprehensive background on plate and shells theory in their book and explained bending (pure and symmetrical) of long, circular, anisotropic and plates having lateral loads, forces in the middle. They also studied rectangular plates (on simply supported and on various edge conditions), plates on elastic foundation and plates of various shapes. Bhat [2] provided natural frequencies of rectangular plates on clamped, simply supported and combination of simply supported and free edges by applying beam characteristic orthogonal polynomials in the Rayleigh Ritz method and showed that when some edges of plate are free, the present method acquires superior result for lower modes. Chakraverty and Petyt [3] discussed transverse vibration of elliptic and circular plates on clamped, simply supported and free boundary using two-dimensional boundary characteristic orthogonal polynomials in Rayleigh Ritz method and evaluated first five natural frequencies for various combinations of non homogeneity and aspect ratios of the ellipse. Li [4] applied Rayleigh Ritz method to analyze the modal characteristics of a rectangular plate with general elastic supports alone its edges and provided numerical examples to demonstrate the accuracy and convergence of the current solution. Ranji and Shahbaztab [5] analyzed free vibration of non homogeneous and orthotropic plate resting on a Pasternak type of elastic foundation by using Rayleigh Ritz method and provided the effect of foundation, density and non homogeneity parameters on natural frequency. Singh and Sexena [6] applied Rayleigh Ritz method to study the transverse vibrations of tapered skew plates with different combinations of boundary conditions and obtained first three modes of frequency and mode shapes. Sharma et al. [7, 8] studied the natural vibration of tapered (exponential and circular variation in thickness) square plate with non homogeneity (variation in

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Vibration of rectangle plate with variable density and Poisson's ratio

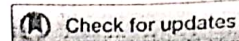**Amit Sharma[1], Vijay Kumar[2], Reeta Bhardwaj[3]**
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Abstract. The effect of variation in density and Poisson's ratio is examined, on the vibration of rectangle plate with linear variable thickness. Bi parabolic temperature effect on the plate is also studied and vibrational modes of rectangular plate is calculated by using Rayleigh Ritz method. Authors also compared the present finding with the published results.

Keywords: vibration, density, Poisson's ratio, variation.

1. Introduction

Isotropic rectangle plate is used in various engineering like civil, mechanical, automobile, aerospace and aircraft engineering. Due to it's wide applications, it is required to know the vibration characteristics of isotropic rectangular plates. The plates made of non-homogeneous material along with variable thickness has significant impact rather than the homogeneous and uniform plates.

An excellent study related to plate vibration, on different edge conditions is given in [1-7]. A finite layer method [8] is used to developed three dimensional linear and small deformation solution for the vibration of rectangular plate on different boundary conditions. The mean square bending moment of a rectangular plate has been discussed in [9]. Rayleigh Ritz technique is used to calculate vibrational frequency of non-homogeneous trapezoidal plate [10] on clamped and simply supported edge condition. The effect of rotary inertia [11] on vibration of rectangular plate with central cutout is studied, using first order shear deformation theory. Forced vibration of orthotropic circular plate with linear variation in thickness, resting on elastic foundation is discussed in [12]. The effect of axial tension, viscosity coefficients and ratio of length-to-depth is studied on transverse vibration of viscoelastic Timoshenko beam columns [13]. Vibration of square and skew plate [14, 15] is discussed with variation in thickness, density and temperature using Classical plate theory. The effect of circular variation in thickness and Poisson's ratio on frequency of square plate is presented in [16]. Vibration of circular plate with parabolic thickness, exponential variation in density and Young's modulus is discussed in [17] using Ritz method. The effect of various plate parameters [18, 19] on vibration of skew and rectangular plate is presented, on clamped edge, using Rayleigh Ritz method. The temperature effect on vibration of rectangular plate made of non-homogeneous material, with variable thickness, is discussed in [20, 21] using Classical plate theory.

The present paper provides the effect of variation in density as well in Poisson's ratio on frequency parameter of the plate. Authors also computed the effect of thickness and temperature on frequency. A comparison of frequency with [20] and [21], with respect to thermal gradient is also given, to validate the finding of the present study.

2. Analysis

Consider a thin rectangular plate with length a, breadth b, thickness l, density ρ and Poisson's ratio ν referred to cartesian coordinates (ζ, ψ).

The maximum kinetic energy of the plate is given by:

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Natural vibration of skew plate on different set of boundary conditions with temperature gradient

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Abstract. A study is carried out to analyze the natural vibration of non-uniform skew (parallelogram) plate made up of non-homogeneous material on different edge conditions, namely clamped (C), simply supported (S) and free (F), using Rayleigh Ritz method. The thickness and Poisson's ratio of the plate varies circular in one dimension, while the temperature variation on the plate is viewed to be parabolic in nature. Natural frequencies have been obtained for different combinations of structural parameters involve in the study. The results are compared with the available published results from the open literature.

Keywords: natural vibration, skew plate, parabolic temperature, different boundary conditions.

1. Introduction

In order to design an accurate structure, determination of natural frequencies and mode shape are essential. The main aim of the researchers and scientists is to optimize the vibration, for the better performance of the mechanical structures. A significant work about the study of vibrational characteristics of plate has been reported.

A comprehensive study about bending of long, circular, anisotropic plate, plates having lateral loads and forces in the middle on plates and shells has been discussed in [1]. Buckling and bending of thin plates and shells are presented in [2]. Natural vibration of homogeneous, isotropic thin annular and circular plates with variable distributions of parameters by using Green's function and Neumann series has been discussed and presented in [3, 4]. Vibrations of functionally graded material (FGM) rectangular plates with porosities and moving in thermal environment by using von Kármán nonlinear plate theory is discussed in [5]. A detailed study about the vibration of plates (square, rectangle, parallelogram, triangle and circular) is discussed and lots of results are presented for homogenous and uniform plates in [6]. A modeling of non-uniform rectangular plates with various cutouts has been discussed in [7] to analyze the free vibration of plates with variable thickness. An approximate method using Green function is presented in [8] to analyze the free vibration of thin and moderately thick rectangular plates with arbitrary variable thickness. Natural vibration of square plate with linear variation in thickness, circular variation in density and exponential variation in Poisson's ratio along with parabolic temperature variation on clamped edges is studied and first two modes of vibration is evaluated in [9]. Thermal effect on vibration properties of double layered nanoplates at small scale has been studied in [10]. Free vibration of non-homogeneous parallelogram plate with variable thickness under temperature variation is studied and results for first two modes of vibration is presented in [11, 12]. Natural vibration of parallelogram plate with exponential variation in thickness, parabolic variation in density and temperature on mixed edge conditions is studied in [13]. Time period [14] for frequency parameter of clamped rectangle plate is calculated on various plate parameters using Rayleigh Ritz method.

In this study, authors examine the behavior of vibrational frequency of parallelogram plate with circular variation in thickness and Poisson's ratio on five edge conditions. The present study also shows the effect of temperature variation on frequency modes. All the obtained results on

Modelling on vibration of skew plate with thickness and temperature variation

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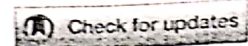[2]Department of Mathematics, Sandip University, Nashik, Maharshtra, India
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Abstract. The present model describes the vibrational analysis of skew (parallelogram) plate made up of non-homogeneous material with variable thickness and temperature on clamped edges. One dimensional thickness and two-dimensional temperature variation is taken into consideration. The non-homogeneity of the plate varies circular in one dimension. The governing differential equation of motion for vibration analysis is solved by using Rayleigh Ritz technique and time period is calculated for the combination of different variation of plate parameters. The obtained results are presented in tabular form.

Keywords: vibration, linear variation, circular variation, thickness.

1. Introduction

Non-homogeneous plate with variable thickness is widely used in structural applications because of their high strength, light weight, and having higher stiffness. Therefore, in order to make good structural applications, it is required to study vibration characteristics of such plates. Many researchers have been worked in this direction and applied various method to solve vibration problem.

Ritz variational method [1] is applied to solve vibration problems of skew plates on different edge conditions and natural frequencies, modes shape is obtained for side ratio and skew angle. Natural vibration of skew plates [2] is presented on eight edge conditions by using the new version of differential quadrature method (DQM). Vibrational analysis of several laminated composite doubly-curved shells, singly-curved shells and plates with variable thickness is analyzed using generalized differential quadrature (GDQ) method [3]. Differential quadrature method (DQM) is used to study the effects of thickness-to-length ratio, volume fraction index, temperature, geometrical shape, and the boundary conditions on the frequency parameters of the functionally graded (FG) quadrilateral plates [4]. The vibrational characteristics of the functionally graded (FG) quadrilateral microplates [5] are investigated by using modified strain gradient theory (MSGT) on different boundary conditions. Free vibration analysis of functionally graded (FG) rectangular plates [6] on simply supported and clamped edge conditions under temperature field is studied and natural frequencies are obtained by Ritz method. Vibrational analysis of two types of functionally graded material (FGM) sandwich plates [7] with nonlinear temperature variation along with thickness is presented by using finite element (layer wise) formulation. Vibration of skew plates [8] with large skew angle is studied by using moving least square Ritz (MLS-Ritz) method and the results are obtained for rhombic plates on various edge conditions. Free vibration analysis of thin laminated skew plates [9] on clamped edges is investigated by using finite strip transition matrix method. Free vibration of rectangular and skew multilayered plate [10] are presented by using variable-kinematic Ritz method on different boundary conditions and evaluated convergence and accuracy of method. The transverse vibrations of skew plates [11] with variable thickness on different combinations of boundary conditions is presented by using Rayleigh Ritz method. The finite strip method [12] is employed to study the free vibration of skew orthotropic plates, with two opposite edges simply supported and the other two edges are free.

6

RNA targeting by an anthracycline drug: spectroscopic and in silico evaluation of epirubicin interaction with tRNA

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RNA targeting by an anthracycline drug: spectroscopic and *in silico* evaluation of epirubicin interaction with tRNA

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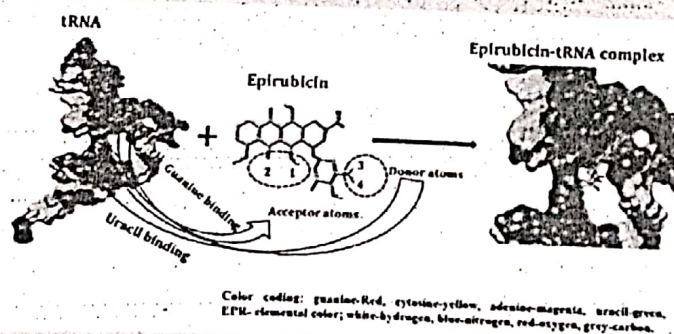
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ABSTRACT

Anthracyclines are putative anticancer agents used to treat a wide range of cancers. Among these anthracyclines, epirubicin is derived from the doxorubicin by the subtle difference in the orientation of C4-hydroxyl group at sugar molecule. Epirubicin has great significance as it has propitious anticancer potential with lesser cardiotoxicity and faster elimination from the body. The present study is done to understand the molecular aspect of epirubicin binding to tRNA. We have used various spectroscopic techniques like Fourier transform infrared spectroscopy (FTIR), absorption spectroscopy and circular dichroism to illustrate the binding sites, the extent of binding and conformational changes associated with tRNA after interacting with epirubicin. From infrared studies, we infer that epirubicin interacts with guanine and uracil bases of tRNA. Results obtained from infrared and CD studies suggest that epirubicin complexation with tRNA does not result in any conformational change in tRNA structure. Binding constant $(2.1 \times 10^3 \text{ M}^{-1})$ calculated from the absorbance data illustrates that epirubicin has a weak interaction with tRNA molecule. These spectroscopic results like the binding site of epirubicin and binding energy of epirubicin-tRNA complex were also verified by the molecular docking. Results of the present study provide information that aids in the development of efficient RNA targeted drugs from the existing drugs by certain chemical modification in their structure resulting in lesser side effects and better efficacy.

Color coding: guanine-Red, cytosine-yellow, adenine-magenta, uracil-green, EPR- elemental color; white-hydrogen, blue-nitrogen, red-oxygen, grey-carbon.

1. Introduction

The detailed study on understanding the interaction mechanism between ligand and nucleic acid is a fascinating area of research. The motivation behind studying the interactions among drug-nucleic acid is the aspiration to decipher drug action at a molecular level. Several anticancer drugs have been developed which possess the property of binding specifically to DNA (Afzal, Al-Lohedan, Usman, & Tabassum, 2019; Bandyopadhyay et al., 2017; Demeunynck, Bailly, & Wilson, 2006; Froehlich, Mandeville, Weinert, Kreplak, & Tajmir-Riahl, 2012; Gao, Sriram, & Wang, 1993; Hadian Rasanani et al., 2018; Hurley, 2002; Moradi, Khorasani-Motlagh, Rezvani, & Noroozifar, 2019). There are various proposed mechanisms by which these drugs are known to exert their biological activity which includes intercalation of drug between DNA strands, binding to grooves, crosslinking between DNA strands (Chaires, 2006; Fiebig, Wan, Kelley, Barton, & Zewail, 1999; Hamilton & Arya, 2012; Karami, Mehri Lighvan, Farrokhpour, Dehdashti Jahromi, & Momtazi-borojeni, 2018; Kosiha, Parthiban, Ciattini, Chelazzi, & Elango, 2018; Lyles & Cameron, 2002; Mansouri-Torshizi, Zareian-Jahromi, Abdi, & Saeidifar, 2018; Moradi, Khorasani-Motlagh, Rezvani, & Noroozifar, 2018; Patra, Paul, Sepay, Kundu, & Ghosh, 2018; Rajski & Williams, 1998; Shahabadi, Shadkam, & Mansouri, 2018). This molecular level understanding of drug binding modes has significantly resulted in the development of more efficacious drugs.

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PAPER

Revisiting the physiochemical properties of Hematite (α-Fe$_2$O$_3$) nanoparticle and exploring its bio-environmental application

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VIBRATION FREQUENCIES OF A RECTANGULAR PLATE WITH LINEAR VARIATION IN THICKNESS AND CIRCULAR VARIATION IN POISSON'S RATIO

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The frequency for the first two modes of vibration of a nonhomogeneous tapered rectangular plate is calculated under a bi linear (i.e., linear along both the axes) temperature field. For consideration of the nonhomogeneous material, the author assumed circular variation in Poisson's ratio. Tapering in the plate is assumed to be linear in one direction. The results are calculated for different values of plate parameters and presented with the help of graphs. Comparison of the results is also given, to support the results of the present study.

Keywords: rectangular plate, circular variation, linear variation, Poisson's ratio

Symbols used

a, b	–	length and breadth of plate, respectively
ζ, ψ	–	coordinates in plane of plate
a/b	–	aspect ratio
M_ζ, M_ψ	–	bending moment intensities in ζ and ψ directions
$M_{\zeta\psi}$	–	twisting moment intensity
Y	–	Young's modulus
D_1	–	flexural rigidity
$\phi(\zeta, \psi, t)$	–	deflection of plate
$\Phi(\zeta, \psi)$	–	deflection function
ρ	–	mass density per unit volume of plate material
$t, T(t)$	–	time and time function
l	–	thickness of plate
m	–	nonhomogeneity constant
α	–	thermal gradient
β, λ	–	tapering and frequency parameter
ν	–	Poisson's ratio

1. Introduction

The most of engineering structures such as rockets, missiles and nuclear reactors are working under sufficient temperature fields. Due to this temperature field, these structures undergo some vibrations. The excess of vibration causes system failure or its less efficiency. Therefore, scientists and engineers are very much keen to optimize the vibrations of structures. For this, they study the dynamic behavior of plates.

Amabili and Carra (2012) studied (experimentally) forced vibrations (large amplitude) of a thin rectangular plate (made of stainless-steel) carrying different concentrated masses. They

Ved Prakash*, Sunita Kumawat and Priti Singh

Design and Analysis of Full and Half Mode Substrate Integrated Waveguide Planar Leaky Wave Antenna with Continuous Beam Scanning in X-Ku Band

Abstract: In this paper, substrate-integrated waveguide (SIW) and half mode substrate integrated waveguide (HM-SIW) periodic leaky wave antennas (LWAs) are presented for the antenna applications. The continuous beam scanning (CBS) is realized by optimizing the unit cell by matching its impedance to the characteristic impedance of the waveguide. This leaky wave antenna is capable of total 60° scanning from −38° to +22.° as the frequency changes from 10.17 GHz to 16.3 GHz with a maximum gain of 11 dBi. Moreover, for further miniaturization, HM-SIW technology is employed in the presented LWA. This LWA is also capable of CBS from −50° to +26° in the frequency band of 10 GHz to 16.5 GHz with a maximum gain of 12 dBi. The final prototypes of the both these antenna are fabricated and measured results are in agreement with the simulated ones.

Keywords: periodic leaky wave antenna, substrate integrated waveguide, half mode substrate integrated waveguide, continuous beam scanning

1 Introduction

One-Dimensional planar leaky wave antenna (LWA), kind of travelling wave antenna, has wide applications in the areas of broadband wireless communications and collision-avoidance radars due to its simple structure, high gain and inherent beam scanning properties in terms of frequency. LWAs are generally composed of waveguides in which a single or double radiators are placed in the unit cell. They are recently being classified into three categories; namely,

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uniform [1, 2], periodic [3–5] and quasi-periodic structures [6, 7]. Uniform and quasi-periodic structures radiates in the forward direction as it radiates from the fundamental space harmonics (n = 0). However, composite right/left handed LWAs belongs to the quasi-periodic structures, which radiates both in the backward to forward direction with fundamental harmonic. The unit cell period for quasi-periodic structures is very small compared to the guided wavelength whereas for periodic LWAs the period is comparable to the guided wavelength. Several types of LWAs have been proposed for beam scanning capability [7–10]. The uniform and periodic LWAs scans only in the forward direction. The broadside radiation is a problem in the conventional LWAs. At broadside frequency, the travelling wave LWA turns into the standing wave antennas. However, with the advent of the composite right/left transmission lines metamaterial [11], continuous beam scanning (CBS) [12] is achieved with the expense of difficulty in fabrication, as the unit cell period is less than $\lambda_g < 4$. Researchers also find out the ways to achieve CBS in periodic LWAs. In [13], quarter distance apart pair of identical elements, can help in achieving CBS. In [14], matching stubs are used for CBS. In [15], unit cell impedance has been matched to characteristic for CBS.

Substrate integrated waveguide (SIW) is one of the most important innovations of the last decade that bridges the gap between planar circuits and metallic waveguides [16]. SIW has advantages of low profile, light weight and can be easily fabricated by standard PCB technology compared to rectangular waveguides. Consequently, SIW has received great interests and various components have been designed using this technology [17, 18]. Half mode substrate integrated waveguide (HM-SIW) for the sake of miniaturization on the transverse side is proposed for the first time [19]. The HM-SIW width and surface area is nearly half compared to SIW while maintaining the fabrication complexity at the same level. Due to the simplicity of these technologies, myriad of leaky wave structures has been proposed on these technologies. In these technologies bulkiness and losses are the great issues to be resolved for LWAs as it moves to the higher frequency range of X and Ku band for satellite.

Petri Net Recommender System to Model Metabolic Pathway of Polyhydroxyalkanoates

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ABSTRACT

Due to the complexity of the metabolic pathways, their modeling has been a great challenge for the researchers. Various mathematical models have been developed and are continuing to be developed to model and study metabolic pathways. In this article, the authors have described Petri nets (PNs) as a recommender system to model one of the metabolic pathways of Polyhydroxyalkanoates. Recommender systems have become an integral part of today's world. Their applications lie in the fields of e-commerce, bioinformatics and many more. Petri nets are one of the promising mathematical tools which can be treated as a recommender system to model and analyze the complex metabolic pathways of various organisms because of the representation of these pathways as graphs. The PN toolbox validates the obtained Petri net model. Polyhydroxyalkanoates, commonly known as PHAs, are biodegradable microbial polyesters and have properties quite similar to commonly used non-biodegradable plastics. Due to their biodegradability, biocompatibility, and eco-friendly nature, they are of biological significance and are used in various applications in wide range of sectors like medical sector, drug delivery, tissue engineering, and many more. The obtained PN model of Polyhydroxyalkanoates has been validated using PN toolbox.

KEYWORDS

Bioplastics, Metabolic Pathways, Petri net Modelling, Petri Nets, Polyhydroxyalkanoates (PHAs), Recommender System

INTRODUCTION

Petri nets are a graphical and mathematical tool used for modelling and studying concurrent, parallel, distributed and discrete event systems (Murata, 1989). Till date they have been successfully applied to various knowledge-based systems like biological networks, communication networks, industrial systems etc. due to their ability to represent any graph-based systems (Murata, 1989; Chaouiya, 2007; Marwan, Wagler & Weismantel, 2011; Reddy, Mavrovouniotis, & Liebman, 1993).

Various approaches have been applied to model the biological networks and Petri nets have been proved to be a promising and effective tool for the modelling and analysis of biological networks. In 1962, a German mathematician Carl Adam Petri first introduced the concept of Petri nets in his Doctoral Dissertation 'Communication with Automata' as a graphical and mathematical tool (Petri, 1966). Several theories from the authors from different backgrounds in different timeframe are available in the literature. For example, most recent proposed theory for 1-safe petri net is Boolean petri net

Catalytic application of zinc complex of oxygen depleted 1,3-bis(pyrazole)-p-tert-butylcalix[4]arene

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ARTICLE INFO

ABSTRACT

In this paper we have described the synthesis and coordination properties of monometallic Zinc complex of oxygen depleted bis(pyrazole)-p-tert-butylcalix[4]arene ligand. We also present the catalytic activity of the Zinc–bis(pyrazole) complex, in acetylation of alcohols and lactide polymerization.

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Introduction

Metal complexes of divalent tetradentate ligands like salen and porphyrin, bearing both hard and soft donors have been extensively used in catalysis [1]. Although, the synthesis of the potential divalent tetradentate calix[4]arene or its derivatives are relatively simple, conveniently providing dozens or even hundreds of grams in one pot, only few metal calixarene catalysts for organic transformations have been reported [2–8]. One likely reason for this inequality is the presence of only hard oxygen donors in the calixarene ligand. Thus, highly oxophilic metal ions form stable complexes at the lower rim making metal complexation relatively inefficient. To circumvent this drawback, very recently, we reported, the first synthesis and complexation studies of calixarene-based ligand having two of its oxygen atoms replaced by sp³-hybridized soft tert-amine donors (Fig. 1) [9]. Catalytic activity of its Ti(IV) complex 3 in various organic transformation has also been studied and found to be superior to the Ti-complex of a parent non-modified calixarene. In continuation of that work, herein, we have reported the synthesis and catalytic activity of Zn-complex of bis-pyrazole calix[4]arene ligand 2.

Result and discussions

We have previously reported the synthesis of bimetallic inclusion complexes when alkyl and aryl ethers of calix[4]arene is treated with $ZnEt_2$ [10]. Surprisingly, when 1,3-Bis(pyrazole)-p-tert-butylcalix[4]arene 2 was treated with $ZnEt_2$ in toluene at room temperature, no complex was formed. Upon subsequent heating at 110 °C; Zn-bis(pyrazole) complex 4 was readily obtained in quantitative yield. Qualitative analysis indicated the formation of a mono-metallic Zn complex, where oxygen of the 1,3-phenols has replaced the two ethyl's of the reagent. Unfortunately, readable crystals could not be obtained for the Zn-bis(pyrazole) complex 4; its structure therefore was confirmed by its ^1H, ^{13}C, ^{15}N NMR, and HRMS data (Scheme 1).

Diffusion NMR studies further confirmed the structure of mono-metallic Zn-complex 4 with the diffusion constant for complex and ligand 0.4926×10^{-5} $cm^2 s^{-1}$ and 0.4979×10^{-5} $cm^2 s^{-1}$ respectively (Fig. 2). Complex 4 was also obtained in good yields when 1,3-bis(pyrazole)-p-tert-butylcalix[4]arene 2 was treated with Zn(N(TMS)$_2$)$_2$ in hot toluene.

The coordination mode in the complex 4 was verified by preparing ^{15}N-labeled equivalent of 2 and 4 and studying their ^{15}N NMR. The NMR spectrum of ^{15}N-labeled 2 shows two doublets at 298.6 (J_{NN} = 12.3 Hz) and 211.8 ppm. The ^{15}N NMR spectrum of 4 exhibits two doublets at 266.2 ppm (J_{NN} = 9.2 Hz) and 213.1 ppm. Comparison of these signals allows the assigning of coordination of nitrogen atoms with metal centre of 4 (Fig. 3) [11].

Among many applications of the novel monometallic complex 4 acetylation of alcohols seemed attractive to us due to their importance in biological system and organic synthesis [12]. In literature, Zn complexes are known to catalyze the acylation of alcohols [13]. Recently, Rebek and co-workers have demonstrated the

ORIGINAL RESEARCH

Synthesis and characterization of oxygen depleted *tert*-amine calix[4] arene ligands and study the effect on sigma non-opioid intracellular protein receptor

Navaneet Chaturvedi[1,2] · Abha Mishra[1] · Varun Rawat[3]

Abstract

This study focuses on the biological prospects of oxygen-depleted calix[4]arene ligands on a protein target. Because of their extensive medical relevance, the oxygen-depleted bis(piperdine) (BPD) and bis(pyrazole) (BPZ) ligands were synthesized and characterized by NMR and mass spectrometry. Furthermore, molecular docking followed by molecular dynamics simulation was utilized to understand the behavior of ligands on selection of sigma non-opiod intracellular receptor (SigNOR) as a suitable protein target. The simulations were carried out by three level of complexity: (1) Apo SigNOR, (2) BPD: SigNOR, and (3) BPZ: SigNOR. The three complex systems were subjected to stability check before detail analysis. From the results of the estimation of binding free energy, it follows that both ligands possess the same free energy of binding which, in turn, suggests their similar role; however, energy components such as Van der waal and electrostatic potential recommend BPZ were identified as a competitive drug on SigNOR. In addition, temporal distribution of the clusters suggests that scattering of the cluster's popularity is a measure of fast structural transitions in both complexes. Current study utilizes modern approach to synthesis, characterization, and simulation of our ligands. This study appropriately highlights the effect of our ligands on SigNOR Protein, which might further be extended to potential in vitro and in vivo bioassay.

Keywords Calix[4]arene · Chemical synthesis · NMR · Molecular docking · Molecular dynamics simulation

Abbreviations

BPD	Bis(piperdine) calixarene ligand
BPZ	Bis(pyrazole)calixarene ligand
MD	Molecular dynamics
NMR	Nuclear magnetic resonance
ns	Nanosecond
ps	Picosecond
RMSD	Root-mean-square deviation
RMSF	Root-mean-square fluctuation
SigNOR	Sigma non-opiod intracellular receptor
VdW	Van der Waals

Navaneet Chaturvedi and Varun Rawat contributed equally to this work.

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Introduction

Knowledge of the three-dimensional (3D) structure of biomolecule and lead compound of low molecular weight guides importantly towards rational drug design. The rapid characterization of the 3D structure of small ligand molecules in solution was facilitated through a novel nuclear magnetic resonance (NMR) spectroscopy strategy [1]. Earlier, calixarenes have been proposed as potential drug candidates by several researchers, while very recent, calixarene derivatives have been described as metal extractants, ios transporters, electrode ionophores, and optical sensors [2–4]. Furthermore, anti-

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Facile synthesis of CuFe$_2$O$_4$ doped polyacrylic acid hydrogel nanocomposite and its application in dye degradation

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ABSTRACT

Polyacrylic acid hydrogel doped with copper ferrite nanoparticles has been prepared and studied for the removal and degradation of organic dye (methylene blue) from wastewater. Phase purity of nanoparticles was confirmed by powder X-ray diffraction and EDX analysis. Raman spectra showed three bands at E$_g$, F$_{2g}$ and A$_{1g}$, attributing the formation of spinel phase with a band gap of 2.12 eV. Hydrogel composite showed an increase in weight by 1771% when soaked in water. Degradation and absorption studies of methylene blue dye solution with copper ferrite nanoparticles as well as hydrogel nanocomposite suggest absorption of dye by hydrogel and degradation with copper ferrite nanoparticles. Such hydrogel nanocomposites could be a promising material for mitigation of water pollution caused by organic dyes discharged by small and medium scale industries.

1. Introduction

Treatment of polluted water caused by industrial waste continues to be a major challenge for Chemists. Organic dyes used by various industries like textiles, printing, pulp mills, food, and plastics cause water pollution. The stability of dye molecules and their resistance towards biodegradation are the main cause of environmental pollution [1,2]. Several technologies have been used for the waste water management which include biological treatment, coagulation/flocculation, ozone treatment, chemical oxidation, ion exchange, photocatalysis, and adsorption [3,4]. The adsorption of pollutant using eco-friendly materials is considered to be superior over other techniques because of their low cost, the simplicity of design, and ease of operation. Dye removal by activated carbon, zeolite, clay, H$_2$O$_2$, sodium hypochlorite and other chemical agents has been widely practiced in the textile industries [5,6]. Superabsorbent polymers (SAP), such as hydrogels containing different types of functional groups, biocompatible and superior absorption capacity have been investigated for their dye removal, drug design, and photothermal properties [7–10]. In recent past, poly(acrylamide)/sepiolite-hydrogel composites, poly(acrylicacid-co-vinyl-2-pyrrolidone)/laponite hydrogel, and polysaccharide-based magnetic nanocomposite hydrogels have been reported for the removal of various dyes [11–13]. The cationic dye molecules are known to escape into the hydrogels matrices due to electrostatic and hydrophilic interactions [14].

Despite having good dye absorption capacity, a major disadvantage of hydrogels is their disposal after use. Hence, degradation of absorbed dye seems to be the optimal solution. Nanomaterials have been used in various fields ranging from materials to medicines [15,16]. Nano-crystalline Copper ferrite (CuFe$_2$O$_4$), have been reported to show significant dye degradation properties and can separate easily due to their magnetic nature. Thus, it was thought worthwhile to explore the absorption and degradation properties of CuFe$_2$O$_4$ incorporated hydrogel poly(acrylic acid-acrylamide-methacrylate) nanocomposite for dye using a selected dye model, methylene blue (MB).

2. Experimental procedure

2.1. Materials

CuCl$_2$·2H$_2$O, FeCl$_3$·6H$_2$O, NaOH, acrylic acid, ammonium persulphate and MB were purchased from CDH Chemicals. N,N'-methylene bisacrylamide was purchased from Sigma Aldrich.

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Visible-Light Photocatalytic Reduction of CO_2 to Formic Acid with a Ru Catalyst Supported by N,N'-Bis(diphenylphosphino)-2,6-diaminopyridine Ligands

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Visible-light photocatalytic CO_2 reduction is carried out by using a Ru[II] complex supported by N,N'-bis(diphenylphosphino)-2,6-diaminopyridine ("PNP") ligands, an unprecedented molecular architecture for this reaction that breaks the long-standing domination of α-diimine ligands. These competent catalysts transform CO_2 into formic acid with high selectivity and turnover number. A proposed mechanism, with combined electron transfer and catalytic cycles, models the experimental rate of formic acid production.

Designing and assembling catalysts that can utilize the energy of visible light to overcome the barriers to reduce CO_2 is an important fundamental and technological challenge. Success in this endeavor requires confronting the inherent stability and low thermodynamic value of CO_2 and would transform this ubiquitous waste product into a valuable feedstock. For example, photocatalytic formation of formic acid, a two-electron reduction product of CO_2, would yield a commodity chemical and a liquid fuel. Furthermore, formic acid has been identified and explored as a potential carrier of dihydrogen.[1,2]

Homogeneous catalysts have been developed for CO_2 reduction under both electrochemical and photochemical conditions.[3–6] Photocatalysis is a particularly appealing approach as it relies on an essentially limitless and clean solar energy source. Photocatalytic systems consist of integrated components that include a photosensitizer (PS) for harvesting the energy of the light, an electron donor (ED) that provides electrons for the reduction, and a catalyst (CAT) that is a site for the transformation of CO_2. To our knowledge, since their discovery in 1985,[7] all of the reported molecular photocatalysts based on Ru[II] have used α-diimine supporting ligands and these species have fallen into two broad groups. One class are bis(α-diimine) species represented by cis-[Ru(N^N)$_2$(CO)$_2$]$^{2+}$ [8–11] and the other are mono(α-diimine) catalysts represented by

cis,trans-[Ru(N^N)(CO)$_2$Cl$_2$].[12–14] Although a variety of substituents on the α-diimine ligands have been productively explored to improve catalyst performance, given the maturity of this field, a broader variation of molecular architecture is required to provide new insights and stimulate new concepts in this field. Ligand variation and discovery are a central challenge in catalysis and expanding Ru-based photocatalysts beyond the restrictions of α-diimine support is certainly warranted. Support for this approach comes from a very recent report on the use of a photocatalytic phosphine-substituted Ru[II] terpyridine complex—trans-[Ru(tpy)(8-quinolyl(diphenyl)phosphine)-(MeCN)]$^{2+}$—that functions as both a photosensitizer and a catalyst for CO_2 reduction.[15,16]

Recently, pincer ligand-supported catalysts of Fe, Co, Ru, and Ir have been shown to have excellent activity and selectivity for hydrogenation of CO_2.[17–23] Pincer-supported ruthenium complexes can catalyze hydrogenation of CO_2 to yield formate, as well as the reverse dehydrogenation reaction.[24–26] Furthermore, the potential of pincer complexes as efficient electrocatalysts for CO_2 reduction under mild conditions has recently been demonstrated for Mn,[27] Ru,[28] and Ir[29,30] complexes. Interestingly, the Ru complex remains in the α-diimine (i.e., bpy) class of catalysts.

With the objectives of discovering new environments for photocatalytic CO_2 reduction and affording new insight into mechanistic aspects of this transformation, we targeted the preparation of new N,N'-bis(diphenylphosphino)-2,6-diaminopyridine ("PNP") pincer complexes of Ru[II]. [Ru(κ^3-2,6-{Ph$_2$PNR}$_2$(NC$_5$H$_3$)}(CO)$_2$Cl$^+$]Cl$^-$ (R=H, Me), are, to our knowledge, the first Ru-based photocatalysts for CO_2 reduction that do not possess α-diimine ligation as well as use a pincer ligand framework.

The direct addition of N,N'-bis(diphenylphosphino)-2,6-di-(methylamino)pyridine to [{Ru(CO)$_3$Cl$_2$}$_2$] in toluene followed by heating at 100°C under N_2 for 16 h led to the new cationic Ru complex [Ru{κ^3-2,6-(Ph$_2$PNMe)$_2$NC$_5$H$_3$}(CO)$_2$Cl]$^+$Cl$^-$ (1$^+$Cl$^-$) as a colorless solid with a yield of 89%. Replacing the starting ligand with N,N'-bis(diphenylphosphino)-2,6-diaminopyridine and following a similar procedure produced the analogous complex, [Ru{κ^3-2,6-(Ph$_2$PNH)$_2$NC$_5$H$_3$}(CO)$_2$Cl]$^+$Cl$^-$ (2$^+$Cl$^-$; Scheme 1). Spectroscopic data and a single crystal x-ray analysis of 1$^+$Cl$^-$ definitively confirmed the identity of this species. As shown in Scheme 1, cation 1$^+$ exhibited a distorted octahedral environment for the Ru[II] center composed of a tridentate, mer-PNP ligand, a CO ligand oriented trans to the pyridyl func-

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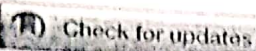
Ultra-small palladium nano-particles synthesized using bulky S/Se and N donor ligands as a stabilizer: application as catalysts for Suzuki–Miyaura coupling†

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Two chalcogenated ligands L1 and L2 containing anthracene core and amine functionality have been synthesized. Both the ligands have been characterized using ^1H and $^{13}C(^1H)$ NMR techniques. The structure of L1 has also been corroborated by single crystal X-ray diffraction. Application of L1 and L2 as stabilizers for palladium nano-particles (NPs) has been explored and six different types of NPs 1–6 have been prepared by varying the quantity of stabilizer. The nano-particles have been characterized by PXRD, EDX, and HRTEM techniques. The size of NPs has been found to be in the range of ~1–2 nm, 2–3 nm, 4–6 nm, 1–2 nm, 1–2 nm and 3–5 nm for 1–6 respectively. The catalytic activities of 1–6 have been explored for Suzuki–Miyaura coupling of phenyl boronic acid with various aryl halides. These NPs showed good catalytic activity for various aryl chlorides/bromides at low catalyst loading (5 mg). Among 1–6, the highest activity has been observed for NPs 1, probably due to their relatively small size and high uniformity in the dispersion. The recyclability of the NPs upto 5 catalytic cycles is a distinct advantage.

Introduction

Palladium-catalyzed C–C coupling reactions are impressive synthetic methods in organic transformations.[1] The tolerance of palladium compounds towards a wide range of functional groups and the easy interchange between Pd(0)/Pd(ii) or Pd(ii)/Pd(iv) oxidation states are mainly responsible for their versatility.[2] Of the various C–C bond-forming reactions, Suzuki–Miyaura coupling is one of the most important methods for the syntheses of diversified and unsymmetrical biaryls (which have numerous applications in synthesis of drugs, natural products, chemicals, advanced material etc.)[3] compared to other coupling reactions, mainly due to the low cost of reagents and ease in handling and removal of reagents and products. The highly efficient Suzuki–Miyaura catalysts include complexes of Pd(ii) with phosphines,[4,5] N-heterocyclic carbenes,[6,7] and organochalcogens[8,9] with an advantage of the ease with which they

can be modified. In order to improve and expand the scope of Suzuki–Miyaura coupling, intensive research efforts are being carried out. In this regard, the development of new catalyst systems with high efficiency and recyclability is an important area that has received particular attention.[10]

In the last few decades, nano-sized palladium particles stabilized with diverse agents, have drawn continuous attraction.[11,12] Nanoparticles play remarkable roles in a variety of fields due to their large surface to volume ratio, reactive surface molecules, and the capability of tuning the properties of material etc.[13–16] High surface to volume ratio of nanoparticles has constrained the researchers to stabilize them by utilizing appropriate stabilizers. The stabilizing ligands play an important role in dictating nanoparticles' size, shape, dispersion, and inter-particle spacing. These ligands also affect the catalytic efficiency, recyclability and solubility of synthesized NPs through ligation. For efficient organic synthesis, generally surfactants, organic ligands, dendrimers, and polymers have been used to stabilize metal nanoparticles.[17–19] The stabilizer molecules generally have functional groups like amine, alcohol, carbonyl or hydroxyl, thiol and phosphine,[20] which limits the catalytic activity because of strong chemisorption.[21] Thus, the stabilizing ligand must be strong enough to stabilize nanoparticles. It must readily allow access of reactant to its surface so that they can be used for multiple reaction cycles. In the absence of a stabilizing agent, there is a possibility of aggregation or precipitation of nanoparticles which results in the loss of

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Bidentate organochalcogen ligands (N, E; E = S/Se) as stabilizers for recyclable palladium nanoparticles and their application in Suzuki–Miyaura coupling reactions

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ABSTRACT

Chalcogeno-substituted secondary amines **L1** and **L2** have been synthesized by the reduction of corresponding imines. Ligands **L1** and **L2** have been characterized using ^1H and $^{13}C\{^1H\}$ NMR spectroscopy. The Schiff base precursors used for the synthesis of **L1** has also been characterized using single crystal x-ray diffraction technique. Both the ligands (**L1** and **L2**) have been used as stabilizers for palladium nanoparticles (PdNPs) **1–4** in two different ratios of Pd:L (1:1 and 1:4). The NPs have been characterized by UV–Vis spectroscopy, powder X-ray diffraction, scanning electron microscopy (SEM), SEM-EDX, and transmission electron microscopy (TEM). The chalcogen donor site showed remarkable role in the stabilization of these nanoparticles. The Pd:L ratio in NPs has been noticed to affect the size and shape of particles and also their catalytic behavior. Size of the NPs has been found to be in a range of 2–3 nm (NPs **1**); 4–5 nm (NPs **2**); 3–4 nm (NPs **3**); and 4–6 nm (NPs **4**). When explored as catalyst, the low loading of these NPs gave significant conversions for the coupling of various aryl halides with phenylboronic acid (Suzuki–Miyaura coupling) in a short reaction time of 3 h. The highest catalytic activity has been observed for Pd NPs **1** (Pd:L ratio 1:1) due to the uniformity in the dispersion of particles. The distinct advantage associated with these NPs (**1–4**) is that they retain catalytic activity after the reaction and are recyclable up to three times. Attempts were made to gain mechanistic insights of catalysis and it was found that both homogeneous and heterogeneous catalytic processes contribute to the catalysis.

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1. Introduction

Palladium-catalyzed Suzuki–Miyaura coupling (SMC) reactions have been used as cutting edge technology [1–3] for many years by chemists. The coupled product of SMC, biaryl derivatives, have been reported to be the part of natural products, pharmaceutical ingredients, agrochemicals and several organic motifs used in material science [4]. SMC has also been considered very important owing to the mild reaction conditions and easy availability of boronic acid derivatives [4a,5]. The less hazardous and non-toxic nature of organoborane, their easy handling and removal of boron-containing by-products in comparison to that of other organometallic reagents is an additional advantage [5,6]. The most common metal used for catalyzing SMC is palladium which has been used either in the form of molecular Pd(II) complex or as nano-sized Pd(0) species [7]. It is believed that real catalytic species is palladium(0) which could be molecular Pd(0) or nanosized palladium species and molecular Pd(II) complexes act only as the dispensers of these species [8]. In case of nanocatalysts, surface area and morphology are important parameters for catalytic performance of palladium NPs when they are used as catalysts or formed in situ during the course of the reaction. The high surface to volume ratio and uniformity in distribution of NPs are expected to enhance the catalytic activity [9].

The synthesis of well defined and mono-dispersed Pd NPs of small size without compromising significantly with the catalytic activity continues to be a challenge. The protecting reagent of NPs should be designed in a way that the activity loss of synthesized NPs is minimal. The ligands used to protect PdNPs result in the reduction of their catalytic activity. Therefore, the role of ligand

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Detoxification mechanism of organophosphorus pesticide via carboxylestrase pathway that triggers *de novo* TAG biosynthesis in oleaginous microalgae

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ABSTRACT

Organophosphorus compounds exhibit a wide range of toxicity to mammals. In this study the effect of malathion on the growth and biochemical parameters of microalgae was evaluated. Three microalgae (*Micractinium pusillum* UUIND2, *Chlorella singulari* UUIND5 and *Chlorella sorokiniana* UUIND6) were used in this study. Among the three algal strains tested, *Chlorella sorokiniana* UUIND6 was able to tolerate 100 ppm of malathion. The photosynthetic pigments, the protein, carbohydrate and lipid contents of microalgal cells were also analyzed. About 90% degradation was recorded in 25 ppm, 50 ppm and 70% was recorded in 100 ppm of malathion by *Chlorella sorokiniana*. A mechanism of degradation of malathion by *Chlorella sorokiniana* is proposed in this study. Activity of carboxylesterase was increased in algal cells cultivated in malathion containing medium which confirmed that malathion degraded into phosphate. Increased amount of Malondialdehye (MDA) indicate the development of free radicals under the stress of malathion which substantialy increase *de novo* TAG biosynthesis, while increased level of superoxide dismutase (SOD), ascorbate peroxidase (APX) and catalase (CAT) suggested their association in scavenging of free radical.

1. Introduction

Malathion is the most widely used organophosphorus pesticide for agriculture throughout the world. These are a potential risk to human health as they can reach the food chain (Low et al., 2013). From the earth pesticides easily accumulate in plants and animals therefore food chain pesticides have received more and more attention (Singh et al., 2012).

In 1937 first organophosphorus insecticide (Tetraethyl pyrophosphate) was developed (Dragun et al., 1984). After the development of Tetraethyl pyrophosphate several other pesticides were also developed and used commercially (Singh and Walker, 2006). In India Malathion is available in form of, a dust, a wet table powder and liquids. Various researchers have reported the toxicity of malathion (Goda et al., 2010; Shan et al., 2009; Singh et al., 2012).

Bulk use or accidental release of organophosphorus pesticides contaminates the surface and ground water (Singh and Walker, 2006). Organophosphorus pesticides are poisonous because of their ability to inhibit acetyl-cholinesterase (Yang et al., 2012). Numerous researchers have reported the role of malathion in a variety of syndromes, hepatotoxicity (Derbalah, 2012; Josse et al., 2014) human breast carcinoma (Kjeldsen et al., 2013), genetic damage (Karami-Mohajeri et al., 2014) and altered hormonal activities (Taxvig et al., 2013). Self-poisoning due to organophosphorus pesticide is one of the major concern in rural regions of the developing countries and responsible for 200,000 deaths per year (Eddleston et al., 2008). The conventional methods for the removal of organophosphorus compounds are very costly and at the same time do not allow a complete solution. Bioremediation appears a promising and effective alternate to this issue.

Microalgae are photosynthetic organisms that can convert light energy into chemical energy just like plants. They have more simple

Reactive magnetron sputtering based synthesis of WO$_3$ nanoparticles and their use for the photocatalytic degradation of dyes

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ABSTRACT

Current study explores the synthesis of WO$_3$ nanoparticles using highly effective novel physical vapour deposition process, reactive magnetron sputtering technique followed by annealing at different temperatures. The characterization of the synthesized samples were carried out by powder XRD, Raman spectroscopy, FE-SEM, TEM, BET, and diffuse reflectance spectroscopy (DRS) to check the crystallinity, morphology, surface area, and optical properties, respectively. Results display that the crystallinity and the crystallite size increases after heating the samples continuously. The morphology was found to be spherical type with high aggregation at low temperature. As-deposited nanoparticles display the highest surface area 66.78 m^2/g and it decreases up to 20.45 m^2/g with increasing the particle size up to 48 nm. The photocatalytic activity of the WO$_3$ nanoparticles was evaluated in the degradation reactions of rhodamine B (Rh B), indigo carmine (IC), and Congo red (CR) in aqueous solution under UV–vis radiation. The highest photocatalytic activity was observed with highly crystalline WO$_3$ nanoparticles and the order of the different organic dyes degradations was: IC > Rh B > CR. The degree of mineralization of organic dyes by WO$_3$ nanoparticles was determined by total organic carbon (TOC) analysis and reaching percentages of mineralization of 76% Rh B, 87% for IC, and 8% for CR for 96 h of lamp irradiation. A proposed mechanism for the photocatalytic activity of synthesized WO$_3$ was investigated in the presence of different scavengers which suggested that mechanism occurs through hydroxyl radicals rather than holes and peroxide radicals.

1. Introduction

Throughout the last decade, transition-metal oxides nanostructures having uniform shapeand size display highly importance in the different areas of intense scientific research and arewidely used in various interesting areas such as catalysis [1], gas sensing [2], pigments in paints and ceramics [3], wastewater treatment [4], organic compounds degradation [5], andphotocatalyst in a large variety of chemical reactions [6]. Among different metal oxides, tungsten (VI) oxide (WO3) is one of the most interesting semiconductor material for thescientific community due to its low processing cost, tuneable band gap, and high solubility inaqueous solutions under acidic conditions. Also, it does not exhibits photo-corrosion activityand gives polymorphism properties. With the polymorphing nature of WO3, it possess twoimportant phases which attract much attention are hexagonal phase (h-WO3) and monoclinicphase (m-WO3). The hexagonal phase exhibits much better interest in gas sensing and variousother applications due to containing open tunnel structure and high interaction properties. Onthe other hand, monoclinic phase exhibits excellent photocatalytic activity under solarirradiation because it exhibits the proper band-gap energy for the adsorption of visible light [7]. Due to these reasons, WO3 has attracted extra attention and researchers have attempted tosynthesize it from a variety of physical and chemical techniques including sol–gel [8], thermal decomposition [9], acid precipitation [10], hydrothermal synthesis [11], and by ion-exchange methods [12]. From all these methods, monoclinic phase with high purity is mostcommonly obtained at room temperature due to thermal stability while hexagonal phase ismostly obtained from the hydrothermal method due to its metastability. In addition, WO3display strong energy band-gap (Eg) of approximately 2.5–2.9 eV range for visible light atwavelength greater than 480 nm, which makes it an attractive candidate for the photocatalyticapplications under solar irradiation [13]. Due to this reason,

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Research article

Phyllanthus emblica fruit extract stabilized biogenic silver nanoparticles as a growth promoter of wheat varieties by reducing ROS toxicity

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ABSTRACT

The present study is focused on the biogenic synthesis of AgNPs (B-AgNPs) using fruit extract of Phyllanthus emblica L and its effect (0, 5, 10, 25, 50 mg/L concentrations) on early seedling growth of two wheat varieties (HD-2967 and DBW-17). The prepared silver nanoparticles were characterized with several techniques such as UV-Vis spectroscopy, powder X-ray diffraction as well as high-resolution transmission electron microscopy. The capping of AgNPs by phytochemicals was confirmed by Fourier transforms infrared (FT-IR) spectroscopy. B-AgNPs, chemically synthesized AgNPs, chemically synthesized AgNPs + 10% fruit extract and AgNO₃ salt were compared for phytotoxicity, based on growth parameters, ROS production, cytotoxicity assay and silver accumulation in two wheat varieties (HD-2967 and DBW-17). These effects were more pronounced in the variety HD-2967 over DBW-17 variety at 10 mg/L B-AgNPs exposure. Root cells viability of treated radicles was studied using Evans blue dye assay which suggest that 10 mg/L B-AgNPs was effective in promoting early seedling growth by decreasing ROS toxicity. Lower accumulation of Ag resulting in higher root cell viability than those of chemically synthesized AgNPs treated seedlings. The findings of the present study clearly indicate that phytochemicals capped AgNPs act as a growth promoter at lower concentrations by delivering a potent antioxidant during early seedling growth as compared to chemically synthesized AgNPs treated wheat seedlings.

1. Introduction

Seed germination and early seedling development are two important phases of crop plants for sustainable agriculture. During seed germination, many biochemical and cellular events trigger the production of reactive oxygen species (ROS) (Wojtyla et al., 2016). The reactive oxygen species such as superoxide radical ($O_2^{\cdot-}$), hydroxyl radical ($\cdot OH$), hydrogen peroxide (H_2O_2), and singlet oxygen ($^1O_2$) are byproducts of many biochemical processes in plants (Sharma et al., 2012). Low levels of ROS are produced in seeds after imbibition to break dormancy and initiate seed germination. A negative impact in the absence of an efficient antioxidant observed on seed germination during seedling growth as high ROS level result in oxidative stress (Kumar et al., 2015). ROS as well

as different plant hormones such as auxin, cytokinin and ethylene, control seed germination and early seedling growth (He et al., 2012). Among these, ROS are key signaling molecule for breaking the dormancy in a concentration-dependent manner. Studies on Oryza sativa and Arabidopsis thaliana have shown that suppression of ROS generation inhibited seed germination (Leymarie et al., 2012). The role of ROS are crucial since low ROS generation can break seed dormancy, while abundant levels can inhibit seed germination as well as seedling growth (Bailly et al., 2008). Therefore, plants have an efficient antioxidant system to fine tune ROS levels for better seedling growth. Exogenous application of antioxidants such as ascorbic acid (ASA) promotes seed germination and seedling growth even under saline stress (Shalata and Neumann, 2001; Wang et al., 2019).

Enhanced potential of biomimetic, silver nanoparticles functionalized *Antheraea mylitta* (tasar) silk fibroin nanofibrous mats for skin tissue engineering

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ARTICLE INFO

ABSTRACT

In the present study, we have successfully prepared tasar fibroin nanofibrous mats using 1-butyl-3-methylimidazolium acetate for skin tissue engineering. The prepared tasar nanofibrous mat was further coated by silver nanoparticles (AgNPs) *in situ* using dandelion (*Tridax procumbens*) leaf extract. The kinetic of silver nanoparticles formation was studied by UV-VIS spectrophotometer. The prepared silver nanoparticles were further confirmed by XRD and TEM. The coating of tasar nanofibrous mat with silver nanoparticles was confirmed by EDX and EDX mapping techniques. The physical, mechanical, antimicrobial and biological properties of these silver nanoparticles coated tasar nanofibrous mat were determined in order to check its suitability for skin tissue engineering and wound dressing applications.

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1. Introduction

A wound is a disruption in natural anatomical structure of skin which may result from mechanical injury, heat, radiation, chemical or terrorist attacks. The wound healing starts immediately after wounding and body is capable to heal these wounds naturally but some time due to deep dermal injury or some impairment in natural healing events body cannot heal wounds adequately [1]. The wound may be acute that heal normally or acute wounds that arrest in phase of wound healing especially in inflammatory phase due to high level of metalloproteinase that causes degradation of extracellular matrix [2]. Several types of strategies have been utilized for wound managements such as negative pressure therapy that is effective for only small wounds while hyperbaric oxygen therapy does not ensure successful healing even after one year [3–7]. Different types of skin substitutes such as autografts, allografts and xenografts have been successfully utilized for wound management but it is also associated with several limitations such as high cost, risk of disease transmission and limit availability of skin tissues in severally burned patients [8,9]. An alternate option to treat such types of wounds are tissue engineered advanced skin substitutes such as 2D films, 3D scaffolds, cryogels, aerogels and nanofibrous mats have been successfully utilized [10]. Among them nanofibrous mats are gaining importance due to the high surface area, porosity

and natural extracellular matrix like architecture [11]. Electrospinning is a promising technique to fabricate fibrous mat having diameter range from submicron to nanorange. These nanofibrous mats have been successfully utilized as advanced therapeutic materials to manage wounds due to high surface area, porosity, good water uptake ability and moist healing, ease permeation of water vapor and gases, breathability, migrations of biomolecules and nutrients that are important for growth of neotissues [12]. Silk, collagen, alginates, chitosan, gelatin and keratin based advanced electrospun materials have been prepared and utilized for wound dressings and regenerative medicine [13–15]. Out of different biomaterials silk has been used in wound management as suture from centuries. Recently, nonmulberry silk fibroin proteins gaining much attention as biomaterials due its excellent biocompatibility, control biodegradability and tuned mechanical properties. The presence of tripeptide (Asp(R)-Gly(G)-Arg(D)) is responsible for integrin mediated cells adhesion because positively charged arginine residue easily bind negatively charged cell surface [13]. Electrospun mats from mulberry fibroin blends have been prepared by various researchers due its solubility in various solvents but only little work has done on the nonmulberry silk fibroin proteins. Due to the high hydrophobic amino acid proportion it is not solubilized in most of solvents in which mulberry dissolve so most of study on nonmulberry silk fibroin proteins is centered on utilization of fibroin proteins extract from gland of silkworm insect [16]. Few research group developed gland tasar fibroin based blend nanofibrous mats for tissue engineering applications [17–19]. Andiappan et al. [20] developed eri and tasar silk

ORIGINAL PAPER

Charge calculation studies done on an end-functionalized double-walled carbon nanotube using MOPAC

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Abstract: Carbon nanotubes functionalized with the appropriate group are important from the point of view of applications of these nanotubes in drug delivery. In this work, we study the charge configuration on the surface of a double-walled carbon nanotube (DWCNT) when it is functionalized with the amidogen group using MOPAC, i.e., molecular orbital package. This kind of a study is performed for a DWCNT for the first time. Taking their electrical properties into consideration, we have functionalized this DWCNT with the amidogen functional group. As nitrogen atom in the amidogen group carries a lone pair of electron, amidogen being electron-releasing group, the addition of this causes the variation in the charge values on the carbon atoms of the DWCNT. Thus, net atomic charge is distributed over the DWCNT system. The effective charge variation is observed close to the carbon atom to which the amidogen group is attached. This charge distribution is then compared with the bare DWCNT case where no external group is attached. The effective charge distribution on the DWCNT surface is observed to be dependent on the mutual length of the constituent walls in DWCNT. Analyzing the charge distribution, the current due to a potential difference applied to the outer CNT would generate sufficient torque to overcome the static and dynamic frictional forces that exist between the inner and outer walls, thereby causing the inner tube to rotate. Application of the charge calculation studies for the nanomotor application of the nanotubes is also discussed.

Keywords: Carbon nanotube (CNT); Single-walled carbon nanotube (SWCNT); Double-walled carbon nanotube (DWCNT); End functionalization; Amidogen (NH_2); Molecular orbital package (MOPAC)

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1. Introduction

Carbon nanotubes (CNTs) are one of the revolutionary outcomes in the field of nanotechnology. CNTs are nowadays a promising subject of research. Despite a lot of researches already done on CNTs, it is still an attraction of researchers' interest. The reason is that CNTs exhibit outstanding and unique physical and chemical properties. Carbon nanotubes can be classified into various categories based on the number of layers as single-walled carbon nanotubes (SWCNT) and multi-walled carbon nanotubes (MWCNTs), and depending on the chirality, these can be classified as armchair, chiral and zigzag. The carbon nanotubes can be described by a chiral vector or roll-up vector "C" as $C = na_1 + ma_2$, where a_1 and a_2 are graphene vectors of honeycomb lattice and m and n are integers. Depending upon the chirality, CNTs can be either semi-conducting or metallic in nature with different sizes of energy gaps, depending on indices (n, m) [1]. The bonds are responsible for the mechanical properties, while bands are responsible for electronic properties. Single-walled carbon nanotubes (SWCNTs) are nanostructures formed from a folded graphene sheet having sp^2-hybridized carbons, with radius of the order of a few nanometers (nm) and length of the order of micrometer (μm). Thus, they possess the simplest geometry as they are single-layered structure.

Because of the extraordinary properties, carbon nanotubes provide a wide range of applications in various fields such as for energy storage, optical electronics, biological engineering, photovoltaic, sensors, ultra-filtration, composite materials and nanodevices [2, 3]. Nanomachines

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